

1-Propene, 1,3-dichloro-

Other names:	1,3-D 1,3-DICHLORO-2-PROPENE 1,3-DICHLOROPROPENE 1,3-DICHLOROPROPYLENE 1,3-Dichloro-1-propene 1,3-Dichloro-1-propene,c&t 1,3-Dichloropropene,c&t 1,3-Dichloropropene-1 1,3-Dichlorpropene 3-Chloroallyl chloride 3-Chloropropenyl chloride D-D92 D-D95 Dedisol C Dorlone II NCI-C03985 NSC 6202 Nemex Propene, 1,3-dichloro- Telone Telone 2000 Telone C Telone II Telone II-B «alpha», «gamma»-Dichloropropylene «gamma»-Chloroallyl chloride Â«alphaÂ», Â«gammaÂ»-Dichloropropylene Â«gammaÂ»-Chloroallyl chloride
Inchi:	InChI=1S/C3H4Cl2/c4-2-1-3-5/h1-2H,3H2
InchiKey:	UOORRWUZONOOLO-UHFFFAOYSA-N
Formula:	C3H4Cl2
SMILES:	ClC=CCCl
Mol. weight [g/mol]:	110.97
CAS:	542-75-6

Physical Properties

Property code	Value	Unit	Source
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gf	30.74		kJ/mol	Joback Method
hf	-19.51		kJ/mol	Joback Method
hfus	12.12		kJ/mol	Joback Method
hvap	31.00		kJ/mol	Joback Method
log10ws	-1.73			Crippen Method
logp	1.978			Crippen Method
mcvol	73.310		ml/mol	McGowan Method
nfpaf	%!d(float64=3)			KDB
nfpah	%!d(float64=2)			KDB
pc	4283.05		kPa	Joback Method
tb	347.06		K	Joback Method
tc	539.68		K	Joback Method
tf	178.33		K	Joback Method
vc	0.281		m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	95.61	J/molxK	347.06	Joback Method
cpg	119.14	J/molxK	507.58	Joback Method
cpg	115.03	J/molxK	475.47	Joback Method
cpg	110.64	J/molxK	443.37	Joback Method
cpg	105.95	J/molxK	411.27	Joback Method
cpg	100.95	J/molxK	379.16	Joback Method
cpg	122.99	J/molxK	539.68	Joback Method
dvisc	0.0002812	Paxs	347.06	Joback Method
dvisc	0.0003545	Paxs	318.94	Joback Method
dvisc	0.0004674	Paxs	290.82	Joback Method
dvisc	0.0006537	Paxs	262.69	Joback Method
dvisc	0.0009911	Paxs	234.57	Joback Method
dvisc	0.0016830	Paxs	206.45	Joback Method
dvisc	0.0033771	Paxs	178.33	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	378.70	K	97.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.53145e+01
Coeff. B	-3.56964e+03
Coeff. C	-4.69710e+01
Temperature range (K), min.	284.52
Temperature range (K), max.	403.83

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C542756&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1735
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating

pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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